1,1,1,2-Tetrachloroethane 630-20-6 | DTXSID2021317

Model Performance

Model	Data

Weighted KNN model

5-fold CV (5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.81	0.55	0.81	0.54	0.71	0.61	

Model Results

Predicted value: 77.2 L/kg

Global applicability domain: Inside

Local applicability domain index: 5.87e-01

Confidence level: 8.63e-01

Nearest Neighbors from the Training Set

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1,1,2,2-Tetrachloroethane

Measured: 79.4 Predicted: 77.8

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Trichloroethylene

Measured: 100 Predicted: 83.1

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1,2-Dibromo-3-chloropropane

Measured: 70.8 Predicted: 84.1

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1,2-Dibromoethane Measured: 51.3 Predicted: 55.8

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1,1,2-Trichloroethane Measured: 77.6 Predicted: 87.6